The applicant has submitted herewith 37 sheets of formal drawings (Figures 1-31C) for submission into the application.

In the claims:

Please amend claims 1-10, 12-16 as shown in the attached clean and marked forms of the pages showing the claims as now pending, pursuant to 37 C.F.R. 1.121(b).

## REMARKS

The applicant responds to the office action dated June 17, 2002, and overcomes each of the office action's grounds for rejection of the claims.

Claims 1-10, 12-16 have been amended. According to an aspect of the invention, a Kekulé structure representation of a chemical structure is analyzed and, based on valence information, a plurality of fixed bond representation candidates are identified for at least a portion of the chemical structure. Further according to the aspect of the invention, at least a subset of the fixed bond representation candidates is evaluated, a selection is made from among the plurality of fixed bond representation candidates based on the evaluation; and fixed bond information is produced based on the selection.

### Claims Not Rejected Under 35 U.S.C. 102 or 35 U.S.C. 103

The applicant has noted that claims 5, 9-10, and 12-14 have not been rejected under 35 U.S.C. 102 or 35 U.S.C. 103. Claims 5, 9-10, and 12-14 have been rejected under 35 U.S.C. 112 only.

### Objections to the Specification/Disclosure

In response to the office action's objections to the drawings, the applicant has submitted formal drawings herewith. No new matter has been added.

The specification has been objected to as having an incomplete "Brief Description of the Drawings" section. The applicant has amended the specification to address the objection, as

shown in attached pages pursuant to 37 C.F.R. 1.121 pertaining to the specification section entitled "Brief Description of the Drawings". No new matter has been added.

In response to a statement in the office action, claim 16 has been amended to recite "practical" as recited in the specification at least at page 7, line 19 and in multiple other instances in subsequent paragraphs.

Rejections Under 35 U.S.C. 112

Claims 1-18 have been rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which the applicant regards as the invention.

The office action states that claims 1-18 are vague and indefinite as to whether they require any type of derivation. The applicant has amended all of the independent claims to make clear that fixed bond information is produced based on the selection already recited in the independent claims. Support may be found in the specification at least at page 5, lines 10-12, at the Summary of the Invention section, at the first and second paragraphs of the Detailed Description section, and at Figs. 6, 8 and accompanying text.

The office action states that claim 10 lacks clear antecedent basis. The applicant has amended claims 9-10 to make clear that a fixed bond representation is produced based on the fixed bond information. Support may be found in the specification at least at the first and second paragraphs of the Detailed Description section, and at Figs. 6, 8 and accompanying text.

The office action states that claims 13-14 lack clear antecedent basis. The applicant has amended claims 13-14 so that claims 13-14 depend from claim 12, which recites a table. Support may be found in the specification at least at page 7, lines 5-10.

Rejections Under 35 U.S.C. 102

Claims 1, 2, 4, 6-8, 11, and 15-18 have been rejected over Organic Chemistry, Third Edition, by Robert Thorton Morrison and Robert Neilson Boyd, copyright 1973 by Allyn and Bacon, Inc. ("the Organic Chemistry reference") at page 261 and/or page 1011.

All of the independent claims have been amended to recite that the analysis is directed to a Kekulé structure representation. Support may be found in the specification at least at page 1, lines 14-16, at Fig. 1 and accompanying text, and at other figures and accompanying text illustrating Kekulé structure representations pursuant to page 1, lines 14-16. Dependent claims 4-10, 12, and 15 have been amended for consistency with the amended independent claims.

The Organic Chemistry reference is an organic chemistry textbook that discloses chemistry principles of valence and bonding. Organic Chemistry reference page 261 ("Page 261") is directed to hydration of alkynes/tautomerism, and Organic Chemistry reference page 1011 ("page 1011") is directed to structure of pyridine.

All of the claims require, among other things, both (1) analyzing a Kekulé structure representation of a chemical structure, and (2) identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. Such analysis and identification as recited in the claims is not taught or suggested in pages 261 and 1011 and is not taught or suggested in any of the cited references.

The Background of the Invention section of the application (at least at page 1, lines 14-16) makes clear that it is known that alternating single and double bonds of the classical depiction can be replaced by all single bonds, adorned by a circle or arc, in a Kekulé structure representation. However, with respect to analysis of a Kekulé structure representation, neither page 261 nor page 1011 teaches using valence information as a basis for identifying fixed bond representation candidates for at least a portion of a chemical structure for which a Kekulé structure representation has been analyzed, as required by all the claims. Moreover, neither page 261 nor page 1011 discloses or suggests the additional elements of evaluating at least a subset of

the fixed bond representation candidates, selecting from among the plurality of fixed bond representation candidates based on the evaluation, and producing fixed bond information based on the selection, all of which are required by all of the claims. For example, neither page 261 nor page 1011 offers even a hint as to how to evaluate and select from among a plurality of fixed bond representation candidates in the context of a Kekulé structure representation, much less an analysis of a Kekulé structure representation.

Rejections Under 35 U.S.C. 103

Independent claim 3 has been rejected under 35 U.S.C. 103 over pages 261 and 1011. However, amended claim 3 is patentable for at least the same reasons stated above with respect to amended claims 1-2.

Remaining Claims

The remaining claims not specifically cited above are patentable for at least the same reasons stated above.

The applicant submits that the application is in condition for allowance, which action is requested.

The Examiner is encouraged to telephone the undersigned to discuss any matters in furtherance of the prosecution of the subject application.

The Commissioner is hereby authorized to charge any fee deficiency, or credit any overpayment to our Deposit Account No. 08-0219.

Respectfully submitted,

Dated: December 17, 2002

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**Replacement Pages for Claims 1-18**
**(MARKED TO SHOW CHANGES)**

1. A method for use in deriving fixed bond information, comprising:

analyzing a [delocalized] Kekulé structure representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates; [and]

selecting from among the plurality of fixed bond representation candidates based on the evaluation; and

producing fixed bond information based on the selection.

2. A system for use in deriving fixed bond information, comprising:

an analyzer analyzing a [delocalized] Kekulé structure representation of a chemical structure;

an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

an evaluator evaluating at least a subset of the fixed bond representation candidates; [and]

a selector electing from among the plurality of fixed bond representation candidates based on the evaluation; and

a producer producing fixed bond information based on the selection.

3. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a [delocalized] Kekulé structure representation of a chemical structure;

identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluate at least a subset of the fixed bond representation candidates; and

select from among the plurality of fixed bond representation candidates based on the evaluation; and

produce fixed bond information based on the selection.

4. The method of claim 1, wherein at least a portion of the [delocalized] Kekulé structure representation describes a monocyclic ring system.

5. The method of claim 1, wherein at least a portion of the [delocalized] Kekulé structure representation describes a polycyclic ring system.

6. The method of claim 1, wherein at least a portion of the [delocalized] Kekulé structure representation describes a ring system with a hetero substitution pattern.

7. The method of claim 1, wherein at least a portion of the [delocalized] Kekulé structure representation describes a non-cyclic system.

8. The method of claim 1, wherein at least a portion of the [delocalized] Kekulé structure representation describes an acyclic system.

9. The method of claim 1, further comprising:

based on the fixed bond information, producing a [including, in the produced] fixed bond representation [,] that includes a pair of opposite charges lacked by the [delocalized] Kekulé structure representation.

10. The method of claim 1, further comprising:

based on the fixed bond information, producing a [including, in the produced] fixed bond representation [,] that includes a pair of radicals lacked by the [delocalized] Kekulé structure representation.

11. The method of claim 1, further comprising:

queuing at least a subset of the candidates by priority.

12. The method of claim 1, further comprising:

using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the [delocalized] Kekulé structure representation.

13. The method of claim 12 [1], wherein the table is configured to allow additional elements and values to be added.

14. The method of claim 12 [1], wherein the table is configured to allow additional elements and values to be added to apply to any chemical element.

15. The method of claim 1, further comprising:

deriving electronic state and valence distributions information together with analyzing the [delocalized] Kekulé structure representation.

16. The method of claim 1, further comprising:

determining whether it is [practicable] practical to produce a fixed bond representation of the chemical structure.

17. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of radicals requirements.

18. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of charges requirements.

**Replacement Pages for Text on Page 2, Lines 17-20 and Page 3, Lines 1-2**

**(MARKED TO SHOW CHANGES)**

Brief Description of the Drawings

[Figs. 1-6, 8, 10, 12, and 15-21 are illustrations of output produced by software.

Figs. 7, 9, 11, and 13-14 are illustrations of computer data.

Figs. 22, 23A-23B, 24, 25A-25C, 26A-26B, 27-30, and 31A-31C are flow diagrams of computer-based procedures.]

Fig. 1 is an illustration of output produced by software showing fixed-bond and delocalized-bond representations.

Fig. 2 is an illustration of output produced by software showing mesomers.

Fig. 3 is an illustration of output produced by software showing a carbene example.

Fig. 4 is an illustration of output produced by software showing an application of dekekulization to the assignment of hydrogenation isomers.

Fig. 5 is an illustration of output produced by software showing the unpredictability of heteroelement hybridization and resulting implicit hydrogen count.

Fig. 6 is an illustration of output produced by software showing the electronic/bonding environments available to a carbon atom with two delocalized attachments.

Fig. 7 is an illustration of computer data listing prevalent atomic environments and corresponding shorthand codes of the form [WXY/Z].

Fig. 8 is an illustration of output produced by software showing the atomic ESVD environments listed in Fig. 7.

Fig. 9 is an illustration of computer data listing control flags.

Fig. 10 is an illustration of output produced by software showing an example of environment development and backtracking for furan.

Fig. 11 is an illustration of computer data illustrating the meanings of bitmask bits.

Fig. 12 is an illustration of output produced by software showing an example of a path marked with atom and bond (underlined) numbers.

Fig. 13 is an illustration of computer data showing various actions possible in a step of an analysis script as shown in Fig. 14.

Fig. 14 is an illustration of computer data showing an analysis script for the strategy for the example of Fig. 12.

Fig. 15 is an illustration of output produced by software showing an example of an external bond being co-opted to serve as an additional internal single bond.

Fig. 16 is a illustration of output produced by software showing first examples relating to procedures disclosed herein.

Fig. 17 is an illustration of output produced by software showing second examples relating to procedures disclosed herein.

Fig. 18 is an illustration of output produced by software showing third examples relating to procedures disclosed herein.

Fig. 19 is an illustration of output produced by software showing fourth examples, including radical structures, relating to procedures disclosed herein.

Fig. 20 is an illustration of output produced by software showing fifth examples, including acyclic examples, relating to procedures disclosed herein.

Fig. 21 is an illustration of output produced by software showing multi-center bonds.

Fig. 22 is a flow diagram of a computer based procedure including an example of a dekekulization procedure.

Figs. 23A-23B are a flow diagram of a computer based procedure including a procedure that is included in an example of the dekekulization procedure and that is provided with information describing a chemical structure.

Fig. 24 is a flow diagram of a computer based procedure including a recursively executed procedure related to the procedure of Figs. 23A-23B.

Figs. 25A-25C are a flow diagram of a computer based procedure including an ESVD assignment procedure.

Figs. 26A-26B are a flow diagram of a computer based procedure including a bond order assignment procedure.

Fig. 27 is a flow diagram of a computer based procedure including a procedure for verifying an atom data construct as complete.

Fig. 28 is a flow diagram of a computer based procedure including a procedure for determining whether a state representing a complete traversal of a path offers a perfect solution.

Fig. 29 is a flow diagram of a computer based procedure including a procedure for calculating an electronic state and valence distribution screening bitmask for an electronic state and valence distribution.

Fig. 30 is a flow diagram of a computer based procedure including a procedure for calculating an atom screening bitmask.

Figs. 31A-31C are a flow diagram of a computer based procedure including a procedure for rating or scoring a state.